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13. ABSTRACT (Maximum 200 words) Treatment of the simultaneous dynamics of electrons and nuclei with full account of electron nuclear coupling has been applied to polymeric chains. Only the highest frequency longitudinal and transverse vibrational modes couples strongly to the electrons. The quantum dynamics of electron transfer at metal surfaces and of the dissociation of diatomic adsorbates have been investigated to construct models of bonding and dynamics at surfaces, and to calculate rates of ion neutralization, and photodesorption times. Electronic charge transfer, leading to ion neutralization, was studied for the system $\text{Na}^+ + \text{W}(110)$ A method has been developed to treat the coupling of the very different time scales present in molecular dynamics for nuclear (slow) and electronic (fast) motions; it has been based on density operators in Liouville space. The photodissociation of CO adsorbed on the Ni(001) surface by visible and UV light has been described using wavepacket dynamics for two coupled potential energy surfaces, including the vibrational degree of freedom of CO. The treatment incorporates dissipation and force fluctuations at the metal surface, within the diabatic electronic representation. Calculations show that dissipation by electron-hole excitation is a dominant mechanism.				
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FINAL TECHNICAL REPORT, 12/1/94-11/30/95

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MOLECULAR SPECTRA AND DYNAMICS AT INTERFACES

PI'S: N. Yngve Öhrn and David A. Micha

**Quantum Theory Project
WM 363, University of Florida
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MAY 15, 1996**

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PART I (Listings)

b. Papers published in refereed journals

1. J.-L. Calais, E. Deumens, and Y. Öhrn, "A Model for Electron Nuclear Dynamics of a Monatomic Chain" *J. Chem. Phys.* **101**, 3989 (1994)
2. R. Longo, B. Champagne, and Y. Öhrn, "Electron Propagator Theory and Application", *Theoretica Chimica Acta* **90**, 397 (1995).
3. J. Morales, A. Diz, E. Deumens, and Y. Öhrn, "Molecular Vibrational State Distributions in Collisions" *Chem. Phys. Lett.* **233**, 392 (1995).
4. A. Diz, Y. Öhrn, and J. R. Sabin, "Dynamic Charge States and Energy Deposition of Swift Helium Ions in Neon." *Nucl. Instr. Meth.* **B96**, 633 (1995).
5. J. Morales, A. Diz, E. Deumens, and Y. Öhrn, "Electron nuclear dynamics of $H^+ + H_2$ collisions at $E_{cm} = 20$ eV.", *J. Chem. Phys.* **103**, 9968 (1995).
6. D. Beksic and D. A. Micha "Electronically Diabatic Quantum Dynamics of Molecular Desorption", *J. Chem. Phys.* **103**, 3795–3808 (1995).

h. Invited presentations

1. Francqui Lecture (Y.Ö.) "Time and Chemistry", at F.U.N.D.P., Namur, Belgium, June 2, 1995.
2. Memorial Symposium for J.-L. Calais, at Uppsala University, Sweden, (Y. Ö.) "Electron Nuclear Dynamics", June 15, 1995.
3. Seminar (Y.Ö.) "Electron Nuclear Dynamics" at the University of Mons, Mons, Belgium, September 13, 1995.
4. Seminar (Y.Ö.) "Coherent States in Molecular Reactive Collisions" the University of Leuven, Belgium September 19, 1995.
5. Seminar (D. A. M.) "Quantum Dynamics of CO Photodissociation from the Ni(001) Surface", Chemistry Department, Univ. of Tennessee (Knoxville), Oct. 2, 1995.
6. Francqui Symposium (Y.Ö.) "Quantum Chemistry; An Overview and a Look to the Future", F. U. N. D. P. , Namur, Belgium October 27, 1995.

j. Awards

N. Yngve Öhrn was awarded the Francqui Professorship (Chaire Francqui Interuniversitaires au Titre Etranger) at Belgian Universities for 1995. This annual award is given in all areas of academe. Dr. Öhrn was the first chemist to receive this honor.

l. Other funding

National Science Foundation "Theoretical and Computational Methods of Quantum Molecular Dynamics", \$ 227,800/(3 years); 2/1/93 to 31/1/96 (extended to 31/1/97); P.I.: D. A. Micha. This grant supports development of methodology and applications to molecular systems different from the ones in the present ONR Grant.

PART II

a. Principal Investigator; N. Yngve Öhm; Co-principal Investigator: David A. Micha

b. Institute phone number: (352) 392-1597

c. Cognizant ONR Scientific Officer: Parbury P. Schmidt

d. Description of the project

This proposal concerns the development and application of theory and computational methods to the spectra and dynamics of molecules adsorbed on solid surfaces. The goals include (a) the development of theory of, in particular, photoelectron spectra and dynamics of adsorbed species with proper account of electronic-nuclear coupling and media effects and (b) the development of the quantum molecular dynamics of atoms and molecules at solid surfaces, and in particular photodesorption and electron transfer at surfaces. The methodologies include electron propagator theory, density matrix and coherent state formulations of quantum molecular dynamics, wavepacket propagation, and molecular dynamics simulations. The research provides information on the structure of adsorbates and helps elucidate mechanisms involved in reactions at solid surfaces, aiding the understanding of adhesion and surface bonding processes. It concerns molecular forces at interfaces, electronic excitation and electron transfer at surfaces, and temperature effects at solid surfaces.

g. Names of research associates and students.

Postdoctoral Research Associates: Keith Runge (100%); Benny Mogensen (50%); Anna Pohl (50%); Graduate Research Assistants: Jorge A. Morales (100%).